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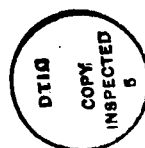
An accurate physical model of a premixed turbulent flame (in the flamelet regime) is that combustion is confined to a thin sheet that can be regarded as a mathematical surface. This surface is convected and bent by the fluid motion, and it propagates normal to itself (relative to the fluid) at the local laminar flame speed. Direct numerical simulations have been performed to examine the important properties of material (i.e. non-propagating) and propagating surfaces in turbulence. The results have been described in seven papers. The straining, curvature and cusp formation of these surfaces has been well characterized.

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1 INTRODUCTION

In the last ten years, great strides have been taken in developing tools to study turbulent reacting flows. Three different approaches to the problem are simultaneously reaching maturity, are elucidating the essential physical processes, and are allowing the prediction of turbulent reactive flows of engineering importance. First, laser diagnostics are being used to extract information undreamt of a decade ago. Second, direct numerical simulations (DNS) of turbulent flows are revealing further information, inaccessible to measurement. And third, stochastic models of turbulent combustion have proved themselves on laboratory flames, and are being extended to the more complex flows of engineering practice. In spite of these strides, there remain fundamental issues on which we are ignorant. In particular, we do not have a clear understanding of the different regimes of premixed turbulent combustion, nor do we have a quantitative understanding of the effect of turbulence on flame sheets.

A straightforward application of DNS to reacting flow problems is to solve for scalar fields representing reactants, products etc. as well as for velocity. While this approach is useful to address some problems, because of the limited range of scales that can be resolved, it does not permit studies in some important parameter ranges. In particular, for premixed flames in the flame-sheet regime, the laminar flame thickness is less than the Kolmogorov scale. The flame sheet could be resolved only if very low Reynolds numbers are used.

Rather than accepting this severe restriction we are using a different approach. A well-tried approach to premixed turbulent flames is to represent the flame as a mathematical surface—a flame sheet—that separates reactants from products. This surface propagates normal to itself relative to the products ahead at a speed w . To a first approximation the propagation speed w is just the laminar flame speed u_L . While many models and theories of turbulent premixed combustion are based on the flame-sheet concept, there is a large number of basic unanswered questions.

In the first half of the project, attention was focused on material surfaces which, by definition, do not propagate relative to the fluid ($w = 0$). Many interesting and important questions concerning the deformation of material surface elements have been answered. In the second half of the project, attention was focused on propagating surfaces ($w > 0$).

In the next section the accomplishments are summarized. In appendix A, the abstracts of the seven papers written during the project are given.

2 ACCOMPLISHMENTS

2.1 Straining on Material Surfaces

A study of the effects of straining on material surfaces has been completed: the results are reported in the paper "Straining and Scalar Dissipation on Material Surfaces in Turbulence: Implications for Flamelets." Some of the prominent findings are:

- the area of a material surface doubles every $2\frac{1}{2}$ Kolmogorov time scales.
- with 80% probability the net straining on a surface element is positive (i.e. extensive); with 50% probability both principal strains (in the plane of the surface) are positive; with less than 2% probability are both principal strains negative.
- a sufficient condition for a premixed flame sheet to remain close to an initially coincident material surface is $w \leq u_\eta$, where w is the laminar flame speed and u_η is the Kolmogorov velocity scale.
- the joint pdf of strain-rate and scalar dissipation has been obtained (which is relevant to turbulent diffusion flames).

These results have been obtained from $(128)^3$ simulations at four Taylor-scale Reynolds numbers from $R_\lambda = 38$ to $R_\lambda = 93$. It is found that none of the statistics investigated (when normalized by the Kolmogorov scales) shows a Reynolds-number dependence. This is in marked contrast to the findings of an earlier study of Lagrangian velocity and acceleration statistics.

2.2 Curvature of Material Surfaces

The DNS code was extended to enable the curvature of material and propagating surfaces to be extracted from the simulations. Along side the Eulerian turbulence simulations, the properties of a large number ($\sim 4,000$)

of infinitesimal surface elements are calculated. These properties are: position; area amplification; unit normal; and the two principal curvatures. The evolution of these properties for each element is determined by a set of ordinary differential equations. These equations contain the first and second spatial derivatives of the Eulerian velocity field. Algorithms (based on cubic splines) have been developed to extract, accurately, the velocity derivatives; and algorithms (based on Runge-Kutta) have been developed to integrate the ordinary differential equations.

Results on the curvature of material surfaces have been obtained from 64^3 simulations. The main results are:

- as time evolves, the mean-square curvature M appears to tend to a stationary distribution. (M is defined by $M = \frac{1}{2}(k_1^2 + k_2^2)$, where k_1 and k_2 are the principal curvatures. The radii of curvatures are $R_1 = 1/k_1$ and $R_2 = 1/k_2$.) But this distribution is such that the mean $\langle M \rangle$ does not exist (loosely, $\langle M \rangle$ is infinite).
- Let $R \equiv M^{-1/2}$ be the mean radius of curvature. It is found that the pdf of R is uniform for small R (i.e. $R < \eta$). This means (loosely) that all radii of curvature $0 \leq R < \eta$ are equally likely. This finding is contrary to conventional wisdom which holds that radii of curvatures below the Kolmogorov scale are improbable.
- It is found that surface elements with large curvature are nearly cylindrical in shape: $|R_2|$ is typically ten times larger than $|R_1|$.

2.3 Material Element Deformation

In Girimaji & Pope (1989b) the previous studies of material surface elements are extended in two ways: first, additional important statistics are reported; and, second, material line and volume elements are also considered. The major findings are now itemized:

- The growth rates of the line and surface elements are significantly less (by a factor of about 3) than previous estimates.
- The smaller growth rates are due to the poor alignment between material elements and the turbulent straining motions. The lack of alignment is caused both by the action of vorticity to rotate the elements,

and because the principal axes of the strain-rate rotate quite rapidly. In other words, contrary to conventional wisdom, we find that strain is fleeting rather than persistent.

- An initially spherical infinitesimal volume element is deformed by the turbulent straining into an ellipsoid. The most probable shape of this ellipsoid is like a squashed cigar—one axis is extended, another equally compressed, while the third remains (approximately) unchanged.

2.4 Stochastic Model for Velocity Gradients

Any quantity related to material element deformation—the straining on a material surface, for example—can be calculated from the velocity-gradient time series following a fluid particle. Thus the study of material element deformation described in the previous subsection was performed using the velocity-gradient time series obtained from DNS.

We have devised a computationally-simple stochastic model for the velocity-gradient time series that reproduces the major statistics of the DNS time series. This stochastic model can be used in turbulent combustion models to calculate the strain rate on the flame sheet etc.

The stochastic model (fully described and tested by Girimaji & Pope 1989a) is a tensor-valued diffusion process. Thus it is a Markov process with continuous sample paths. The drift and diffusion coefficients in the model have been determined—partly analytically, partly empirically—by requiring that the most important statistics of the process match those obtained from DNS. Typically the model is accurate to within 15%.

2.5 Propagating Surfaces

The material surfaces described so far represent flame sheets only in special limits. In the context of premixed flames, the limit is $u_L/u_\eta \rightarrow 0$, where u_L is the laminar flame speed and u_η is the Kolmogorov velocity scale.

We have completed a study of propagating surfaces, with propagation speeds u_L of $u_L/u_\eta = 0, \frac{1}{4}, 1, 4, 16$ (Girimaji & Pope 1990c). The study of propagating surfaces ($u_L > 0$) is much more difficult than that of material surfaces ($u_L = 0$), because of cusp formation. That is, the curvature of a surface element can become infinite in finite time.

The first difficulty to be faced is to devise an accurate and stable numerical algorithm that can calculate the surface properties up to the point or cusp formation. This requires special consideration of the singularity (i.e. the cusps). Such an algorithm has been devised. It is second-order accurate, and reduces to an exact analytic solution as the singularity is approached.

Because of the formation of cusps, the time series of surface properties are finite in duration, and they are inherently non-stationary. Thus the second difficulty is the analysis of these time series—as compared to the stationary time series of arbitrarily long duration for material surfaces.

The results confirm expectations. For example, the Lagrangian time scales and the straining on the surface decrease with increasing u_L/u_η . The precise variation of these statistics is of fundamental importance to theoretical questions of premixed flame propagation. Also as expected, the mean time to cusp formation decreases with increasing u_L/u_η .

3 PUBLICATIONS

P.K. Yeung, S.S. Girimaji and S.B. Pope (1990) "Straining and scalar dissipation on material surfaces in turbulence: implications for flamelets," *Combustion and Flame* **79**, 340-365.

S.B. Pope, P.K. Yeung and S.S. Girimaji (1989) "The curvature of material surfaces in isotropic turbulence," *Physics of Fluids A*, **1**, 2010-2018.

S.S. Girimaji and S.B. Pope (1990a) "A stochastic model for velocity gradients in turbulence," *Physics of Fluids A*, **2**, 242-256.

S.B. Pope (1990) "Computations of turbulent combustion: progress and challenges," Invited Plenary Lecture, Twenty-Third Symposium (International) on Combustion, The Combustion Institute (to be published).

S.S. Girimaji and S.B. Pope (1990b) "Material element deformation in isotropic turbulence," *Journal of Fluid Mech.* **220**, 427-458.

S.B. Pope, P.K. Yeung and S.S. Girimaji (1990) "Stretching and bending of material surfaces in turbulence," First-prize paper in the 1989 IBM 3090 Supercomputing Competition. (MIT Press, to be published.)

S.S. Girimaji and S.B. Pope (1990c) "Propagating Surfaces in Isotropic Turbulence," submitted to *J. Fluid Mech.*

3.1 Reports

P.K. Yeung, S. Girimaji and S.B. Pope (1988) "Eulerian and Lagrangian statistics from a high-resolution direct simulation of stationary homogeneous turbulence," Cornell Report FDA-88-02.

P.K. Yeung, S. Girimaji and S.B. Pope (1988) "A second direct simulation of stationary homogeneous turbulence at $R\lambda 63$," Cornell Report FDA-88-08.

P.K. Yeung, S. Girimaji and S.B. Pope (1988) "Further direct simulations of stationary homogeneous turbulence at $R\lambda 90$ and 93," Cornell Report FDA-88-19.

4 PERSONNEL

The general level of support has been 15% for the PI, Professor S.B. Pope, and the equivalent of one full-time graduate research assistant (GRA). The GRA's working on the project were:

Dr. P.K. Yeung (Ph.D. January 1989)

Dr. S.S. Girimaji (Ph.D. May 1990)

Mr. S. Subramanian (Ph.D. student).

5 INVENTIONS

None.

APPENDIX

Abstracts of Published Papers

Physics of Fluids A, Volume 2, pp. 242-256, February 1990

A diffusion model for velocity gradients in turbulence

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(Received 7 July 1989; accepted 26 October 1989)

In this paper a stochastic model for velocity gradients following fluid particles in incompressible, homogeneous, and isotropic turbulence is presented and demonstrated. The model is constructed so that the velocity gradients satisfy the incompressibility and isotropy requirements exactly. It is further constrained to yield the first few moments of the velocity gradient distribution similar to those computed from full turbulence simulations (FTS) data. The performance of the model is then compared with other computations from FTS data. The model gives good agreement of one-time statistics. While the two-time statistics of strain rate are well replicated, the two-time vorticity statistics are not as good, reflecting perhaps a certain lack of embodiment of physics in the model. The performance of the model when used to compute material element deformation is qualitatively good, with the material line-element growth rate being correct to within 5% and that of surface element correct to within 20% for the lowest Reynolds number considered. The performance of the model is uniformly good for all the Reynolds numbers considered. So it is conjectured that the model can be used even in inhomogeneous, high-Reynolds-number flows, for the study of evolution of surfaces, a problem that is of interest particularly to combustion researchers.

The curvature of material surfaces in isotropic turbulence

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(Received 3 May 1989; accepted 10 August 1989)

Direct numerical simulation is used to study the curvature of material surfaces in isotropic turbulence. The Navier-Stokes equation is solved by a 64^3 pseudospectral code for constant-density homogeneous isotropic turbulence, which is made statistically stationary by low-wavenumber forcing. The Taylor-scale Reynolds number is 39. An ensemble of 8192 infinitesimal material surface elements is tracked through the turbulence. For each element, a set of exact ordinary differential equations is integrated in time to determine, primarily, the two principal curvatures k_1 and k_2 . Statistics are then deduced of the mean-square curvature $M = \frac{1}{2}(k_1^2 + k_2^2)$, and of the mean radius of curvature $R = (k_1^2 + k_2^2)^{-1/2}$. Curvature statistics attain an essentially stationary state after about 15 Kolmogorov time scales. Then the area-weighted expectation of R is found to be 12η , where η is the Kolmogorov length scale. For moderate and small radii (less than 10η) the probability density function (pdf) of R is approximately uniform, there being about 5% probability of R being less than η . The uniformity of the pdf of R , for small R , implies that the expectation of M is infinite. It is found that the surface elements with large curvatures are nearly cylindrical in shape (i.e., $|k_1| \gg |k_2|$ or $|k_2| \gg |k_1|$), consistent with the folding of the surface along nearly straight lines. Nevertheless the variance of the Gauss curvature $K = k_1 k_2$ is infinite.

Straining and Scalar Dissipation on Material Surfaces in Turbulence: Implications for Flamelets

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Direct numerical simulations of turbulence are used to examine the straining on material surfaces, and the behavior of thin diffusive layers. The results are related to questions arising in the study of turbulent premixed and diffusion flames in the flamelet regime. The simulations are of constant-density, homogeneous, isotropic turbulence, with artificial forcing of the velocity field to maintain statistical stationarity. Taylor-scale Reynolds numbers (R_λ) up to 93 are achieved.

It is found that the total rate-of-strain a in the tangent plane of a material surface is positive (i.e., extensive) with 80% probability. This straining causes the area of the surface to double every 2.5 Kolmogorov time scales (τ_η). A premixed flamelet can be viewed as a surface that propagates at a speed w (i.e., the local laminar flame speed) relative to the fluid ahead. It is shown that the distance z between such a propagating surface and an initially coincident material surface remains small if w is small compared to the Kolmogorov velocity scale. For this case, the statistics of z are characterized.

Subject to certain assumptions, the thin diffusive layers between blobs of fluid of different concentration adopt a self-similar form (at least for small times). It is found that the scalar dissipation χ_0 in the center of these layers is approximately log-normally distributed. The mean thickness of these layers is approximately 2 Batchelor scales, and is less than 5 Batchelor scales with 98% probability. The joint probability density of χ_0 and a shows that χ_0 fluctuates significantly about its quasi-static value based on a (for $a > 0$). The integral time scales of a and χ_0 are found to be approximately τ_η and $4\tau_\eta$, respectively. None of the results obtained shows significant Reynolds-number dependence when normalized by the Kolmogorov scales.

ABSTRACT

COMPUTATIONS OF TURBULENT COMBUSTION: PROGRESS AND CHALLENGES

S.B. Pope

We review the significant progress that has been made in the development and use of turbulent combustion models applicable to practical combustion devices. Recent work has focussed on the development of methods that can treat finite-rate kinetics in a realistic yet tractable way, so that local extinction and related phenomena can be studied. Direct numerical simulation cannot be used for this purpose, because it is computationally intractable; and the potential of large-eddy simulation is far from clear because combustion reactions give rise to a severe closure problem. PDF methods, on the other hand, overcome the major closure problems, and they have been shown to be tractable for complex flows and with realistic finite-rate kinetics.

A simple explanation of pdf methods is presented. It is shown that the single modelled equation for the joint pdf of velocity, dissipation and composition provides a closure for turbulent combustion. Reaction and convection are treated exactly, while the modelling is performed in a Lagrangian setting, by constructing deterministic or stochastic models for the evolution of fluid-particle properties. Examples of recent pdf calculations are described, including those based on four-step mechanisms for methane. Extension of pdf methods to include composition gradients is discussed, with a view to improving the modelling of molecular diffusion.

STRETCHING AND BENDING OF MATERIAL SURFACES IN TURBULENCE

by

Stephen B. Pope, Pui-kuen Yeung
and Sharath S. Girimaji

ABSTRACT

In the study of mixing and reaction in turbulent flows, there are several phenomena that can be usefully described in terms of surfaces. Examples are turbulent flames and the turbulent mixing of different liquids. The most fundamental type of surface is the material surface which, by definition, moves with the fluid. Because of the fluid's turbulent motion and deformation, the surface is continually stretched and bent. In this study numerical simulations have been performed to understand and to quantify these processes.

A pseudo-spectral method is used to solve the Navier-Stokes equations which govern the motion of the fluid. These equations are solved on a 128^3 grid for the simplest possible turbulent flow — statistically stationary, homogeneous, isotropic turbulence. As the results show, the direct numerical representation of a material surface is not feasible: for the surface area grows exponentially (by a factor of 10^{17} over the duration of the simulations); and radii of curvature less than a millionth of the grid spacing arise. Instead an indirect method is used in which ensembles (4-8,000) of infinitesimal surface elements are followed. Statistics of interest are obtained from the stretching and curvatures of these elements.

For the first time, the mean rate of stretching has been determined. It is found that the surface area doubles every $2\frac{1}{2}$ Kolmogorov time scales. (The Kolmogorov time scale is the smallest physical time scale in turbulence.) While this is certainly rapid growth, it is only 40% of theoretical estimates, for reasons that are explained. Hitherto, little has been known about the curvature of material surfaces. The results show that extremely small radii of curvatures arise, as small as 10^{-8} of a Kolmogorov length scale (the smallest turbulent scale). These highly curved elements are found to be almost perfectly cylindrical in shape. Many other more refined statistics have been obtained.

The numerical simulations were performed on an IBM3090-600E, with full exploitation of its vector, parallel and large-memory facilities. A typical run requires a total of 80 CPU hours, but can be completed in 20 hours because all six processors are used in parallel.

Material-element deformation in isotropic turbulence

By S. S. GIRIMAJI AND S. B. POPE

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(Received 9 October 1989 and in revised form 27 April 1990)

The evolution of infinitesimal material line and surface elements in homogeneous isotropic turbulence is studied using velocity-gradient data generated by direct numerical simulations (DNS). The mean growth rates of length ratio (l) and area ratio (A) of material elements are much smaller than previously estimated by Batchelor (1952) owing to the effects of vorticity and of non-persistent straining. The probability density functions (p.d.f.'s) of $l/\langle l \rangle$ and $A/\langle A \rangle$ do not attain stationarity as hypothesized by Batchelor (1952). It is shown analytically that the random variable $l/\langle l \rangle$ cannot be stationary if the variance and integral timescale of the strain rate along a material line are non-zero and DNS data confirm that this is indeed the case. The application of the central limit theorem to the material element evolution equations suggests that the standardized variables $\hat{l} \equiv (\ln l - \langle \ln l \rangle)/(\text{var } l)^{1/2}$ and $\hat{A} \equiv (\ln A - \langle \ln A \rangle)/(\text{var } A)^{1/2}$ should attain stationary distributions that are Gaussian for all Reynolds numbers. The p.d.f.s of \hat{l} and \hat{A} calculated from DNS data appear to attain stationary shapes that are independent of Reynolds number. The stationary values of the flatness factor and super-skewness of both \hat{l} and \hat{A} are in close agreement with those of a Gaussian distribution. Moreover, the mean and variance of $\ln l$ (and $\ln A$) grow linearly in time (normalized by the Kolmogorov timescale, τ_η), at rates that are nearly independent of Reynolds number. The statistics of material volume-element deformation are also studied and are found to be nearly independent of Reynolds number. An initially spherical infinitesimal volume of fluid deforms into an ellipsoid. It is found that the largest and the smallest of the principal axes grow and shrink respectively, exponentially in time at comparable rates. Consequently, to conserve volume, the intermediate principal axis remains approximately constant.

The performance of the stochastic model of Girimaji & Pope (1990) for the velocity gradients is also studied. The model estimates of the growth rates of $\langle \ln l \rangle$ and $\langle \ln A \rangle$ are close to the DNS values. The growth rate of the variances are estimated by the model to within 17%. The stationary distributions of \hat{l} and \hat{A} obtained from the model agree very well with those calculated from DNS data. The model also performs well in calculating the statistics of material volume-element deformation.

Propagating Surfaces in Isotropic Turbulence

September 28, 1990

S.S. Girimaji and S.B. Pope

Abstract

Propagating surface evolution in isotropic turbulence is studied using velocity fields generated by direct numerical simulations. The statistics of tangential strain-rate, fluid velocity, characteristic curvature and area following propagating surface elements are investigated. The one-time statistics of strain-rate and fluid-velocity pass monotonically from Lagrangian values at low propagation speeds to Eulerian values at high speeds. The strain-rate statistics start deviating significantly from the Lagrangian values only for propagating velocities greater than the Kolmogorov velocity scale v_η whereas with fluid-velocity statistics the deviation occurs only for velocities greater than the turbulence intensity u' . The average strain-rate experienced by a propagating surface decreases from a positive value to near zero with increasing propagation velocity. The autocorrelation function and frequency spectrum of velocity and strain-rate scale as expected in the limits of small and large propagating velocities. It is also determined that for the range of propagation velocities considered, an initially plane surface element in turbulence develops a cusp in finite time with probability nearly one. The evolution of curvature is studied using the concept of *hitting time*. Initially plane propagating surfaces end up being almost cylindrical in shape. Highly curved surface elements are associated with negative strain-rates and small surface areas.